Ref. Ares(2023)305723 - 16/01/2023

DELIVERABLE REPORT

Deliverable no. / title:	D8.3 USE CASES
Lead beneficiary:	Fraunhofer SCAI
Nature of deliverable:	Report
Dissemination level:	PU – Public
Due date:	M12 / December 2022

Grant Agreement number:	875489
Project acronym:	SONAR
Project title:	Modelling for the search for new active materials for redox flow batteries
Funding scheme:	H2020-LC-BAT-2019
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Project website:	www.sonar-redox.eu

Disclaimer: This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement no. 875489. This report reflects only the authors' view. The funding agency is not responsible for any use made of the information it contains.

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History			
Date	**Version**	**Partner**	**Comments**
01.11.2020	v0.1	Fraunhofer SCAI	creation

List of Acronyms	
DMP	Data Management Plan
EDP	Exploitation and Dissemination Plan
FAIR	Findable, Accessible, Interoperable and Reusable
GA	Grant Agreement
IEB	Industrial Exploitation Board
ORD pilot	Open Research Data Pilot
WP	Work Package

1 General remarks

Use cases are a technique for capturing, modelling and specifying the requirements of a system. As such, they are a way to verify or even demonstrate the relevance of the tasks set, the correctness of the results and thus the overall usefulness of a tool or technique.

This document contains the use cases proposed after three years of research and development. Depending on the still ongoing further developments and input from end-user feedback, the individual examples may be revised or iteratively refined in the remaining time.

Ultimately, this compilation (or a subset thereof) should serve to illustrate the benefits of the individual services during the final workshop and on the central website so that they can be lead to follow-up projects and the project results can continue to be used after the project is completed. Until then, this document will be updated when necessary.

The following section lists for all work packages a preliminary definition of use cases.

2 Use Case definitions

2.1 Work package 1 – high throughput screening

Use Case	Goal	Task	Sample Input	Tool	Output
screening of reference compounds	demonstrate validity of approach/quality of results	For set of compounds, which are the best posolyte/negolyte combinations with respect to basic cell performace parameters?	reference compounds + default reaction templates (D1.4)	standard workflow + 0D model	OCV + max power densities for resulting potential FB chemistries
screening of vendor compounds	demonstrate speed of technique/provide a survey of commercially available chemistries	search a given vendor data base for FB with > 0.4 V OCV	vendor compounds (eMolecules) + default reaction templates	standard workflow, D1.4	OCV for resulting potential FB-chemistries
screening of derivatives	demonstrate in depth study for a given core structure/customize a core structure	for a given scaffold, which functional groups work best with respect to redox potential and solublity?	virtual library (scaffold + functional groups to be chosen) + default reaction templates	standard workflow	half cell potentials, solubility
screening + ageing	find promising posolyte/negolyte combinations and estimate risk of ageing by formal reaction network	for a given class of compounds, which ones are the best posolyte/negolyte pairs AND are they at risk for ageing?	diverse quinone structures + default reaction templates + reaction templates for known ageing mechanisms	standard workflow + modifications	OCV for resulting potential FB-chemistries, list of potential side products
generate mols + screening	find novel chemistry beyond vendor catalogues	create hypthetical molecules and find best posolyte/negolyte combination wrt OCV.	target properties (e.g. half cell potential)	molecule generator + standard workflow	OCV for novel FB chemistries, synthetic accessibility score
design/ optimization	demonstrate design workflow/optimize absolute current	For a given simulation domain, at which flowrate is the maximum absolute current achieved?	D1.5	workflow for optimizing 3D cell designs, (D1.5)	absolute current as a function of flow rate

2.2 Work package 2 – atomistic simulations

Use Case	Goal	Task	Sample Input	Tool	Output
screening or optimization of organic electrolytes	predict potential degradation reactions and rates	for a given electrolyte composition, use efficient algorithms for the exploration of potential energy surfaces to map out a reaction network	molecular species in the electrolyte	electronic structure program with efficient algorithms for single-ended transition state searches + layers of scripts do drive the exploration	rates of degradation reactions

2.3 Work package 3 – electrode kinetics

Use Case	Goal	Task	Sample Input	Tool	Output
screening/ simulation	demonstrate modeling methodology and simulate the potential evolution	Define target events in a given system and simulate the electrochemistry behavior of targeted compounds in mesoscopic level	Experiments and WP2	kMC model	Steady-state potential of target system and the electrical double layer structure
screening/ simulation	simulate the viscosity of electrolyte with different concentration	Estimate the diffusion coefficient and the viscosity of the electrolyte with given concentration and component	Experiments and literature	kMC model adapted to the mean square displacement approach	effective diffusion coefficient of species and the viscosity of electrolyte
design/ optimisation	demonstrate design workflow / optimise eletrolyte utilisation rate	find optimised parameter set for the geometrical structure of carbon felt electrode, which could maximise the electrolyte utilisation rate	software generation of electrode structure	LBM model and optimisation workflow	optimised fiber electrode structure

2.4 Work package 4 – continuum cell

Use Case	Goal	Task	Sample Input	Tool	Output
fast parameter studies for cell design and operating conditions	develop a robust and computationally efficient 0D cell model for performance predictions	Investigation of sensitivity and effect of operating conditions on the cell performance	Ohmic cell resistance, flow rate, reaction rates, half-cell potentials, …	Mathematica	cell voltage as a function of SoC, current density and other model parameters
characterization of the electrochemical interface	demonstrate validity of the approach	Determine double layer charging effects, Perform parameter identification using atomistic model results (e.g. kMC data) and experimental data	Adsorption energies, Solvation shell sizes, Ionic molar volumes and areas, …	Julia	Double layer capacitance
characterization of macroscopic porous electrode properties	provision of a reduced electrode model that allows for an efficient evaluation of effective porous electrode properties	Optimize simplified porous electrode structures to maximize effective reaction rate for a given energy dissipation	porosity, unit-cell geometry, pore-scale transport numbers (Peclet, Kinetic, ..)	Offline-upscaling procedure: COMSOL Online model evaluation: Julia	effective transport parameters (permeability, diffusivity, dispersion, reaction rate)
flow cell design and optimization of operating conditions	develop and validate a time-dependent, non-isothermal flow cell model that can be used to predict cell performance for a wide range of operating conditions	Cell performance study for different cell geometries and operating conditions	cell geometry, initial and boundary conditions (concentrations, temperature, …), material properties (porosity, electrical conductivity, …)	Julia	cell voltage, spatio-temporal resolution of macro-homogeneous fields (concentration, temperature, …)

design of flow channels and optimization of material properties	develop and validate a spatially resolved 3D cell model for performance predictions	What flow channel structure maximizes the cell performance? What is the optimal choice of materials? What operating conditions maximize the cell efficiency?	3D cell geometry including flow channels, boundary and inflow conditions (concen-trations, temperature, …), material properties, …	COMSOL	cell voltage, spatially resolved velocity, pressure, concentration, temperature fields

2.5 Work package 5 – pore scale models

Use Case	**Goal**	**Task**	**Sample Input**	**Tool**	**Output**
screening of electrode material and chemical system	test promising electrode materials and estimate their performance for different electrochemical systems	scan material and built digital twin and find optimum flow rate, current density, concentration …	microstructure digital twin, chemical system	3D microscale continuum model (half-cell)	microstructural dependency of concentration distribution, half-cell potential, flow
design/optimization	demonstrate topology optimisation on the cell level	optimise cell design for laboratory or small.scale application	geometrical data	Simplified 2D half-cell model and topology optimisation framework within COMSOL	new optimised stuctures

2.6 Work package 6 – stack & system

Use Case	Goal	Task	Sample Input	Tool	Output
hydraulic stack model	to simulate the hydraulic performance of a commercial-size battery stack	The hydraulic stack model mainly considers the electrolyte flow and the associated pressure losses through the active cell areas, channels feeding the cells and the manifolds connected to the channels. The pipes and pumps connected to the stack can also be simulated.	cell number, cell geometry, flow frame geometry, SOC range, currents, total concentrations, flow factor, pipe length, pump efficiency etc.	consulting services using the developed standalone software	flow rates, pressure losses of different components in a stack, pump power, flow distribution
electrochemical stack model	to simulate the electrochemical performance of a commercial-size battery stack	The electrochemical stack model is based on an equivalent resistor network to determine the cell voltages, currents, energy and efficiencies, considering the ion diffusion across the membrane, gassing side reactions and oxidation of ions.	cell number, stack geometry, capacity, SOC range, currents, total concentrations, diffusion coefficients, cell formal potential, resistivity, current efficiency factor etc.	Consulting services using the developed standalone software	electrolyte concentrations, cell and stack voltages, cell + shunt currents resistances, energy, efficiencies

2.7 Work package 7 – holistic

Use Case	Goal	Task	Sample Input	Tool	Output
techno-economic benchmark of different aqueous flow batteries	development of a stand-alone software for the output of cost allocations and as a basis for a possible integration into a Micro-Grid simulation	simple adaptation of an existing techno-economic model filled with input variables to own FB or own input variables and fast output of the resulting relevant cost distributions	basic fitting with more than 40 input variables as mean values of validation measurements carried out in the laboratory	python-based techno-economic model of organic and inorganic aqueous flow batteries	energy and power related costs and their distributions

3 Next steps

- The current definitions will be presented to end-users for evaluation.
- Depending on the assessment, the tasks/scenarios may be revised and/or the examples completed with concrete input and reference data.
- In a later phase, the results are reviewed and assessed again by the end users.
- Proven examples may be presented at an end-user workshop and will be published on the website.